
Program

XXIInd International Symposium on the Jahn-Teller Effect 18th – 22nd August 2014, Graz, Austria

Sunday, 17 August 2014

16:00 – 18:00 Registration Desk opens
REGISTRATION

18:00 – 19:00 Welcome Reception

Monday, 18 August 2014

8:00 – 9:00 **REGISTRATION**

8:50 – 9:00 **Welcome and Opening**

Chair: Wolfgang ERNST

9:00 – 9:45 **Isaac B. BERSUKER** (The University of Texas at Austin)
The Pseudo Jahn-Teller Effect: Special Features, Novel Findings, and Applications (REV1)

9:45 – 10:30 **Vladimir HIZHNYAKOV** (University of Tartu)
Time-dependent Jahn-Teller Problem in Solids: Phonon-Induced Relaxation (REV2)

10:30 – 11:00 Coffee Break

Chair: Hiroyasu KOIZUMI

11:00 – 11:25 **Markus AICHHORN** (Graz University of Technology)
Cooperative effects of Jahn-Teller distortion, magnetism and Hund's coupling in BaCrO₃ (O01)

11:25 – 11:55 **Mihail ATANASOV** (Max-Planck Institute for Chemical Energy Conversion)
Ab initio Studies on the Role of the Jahn-Teller and Renner-Teller Effects in Single Molecule Magnets (INV1)

11:55 – 12:20 **Max SORANTIN** (Graz University of Technology)
Vibronic effects on the steady state current through a molecular ring structure (O02)

12:30 – 14:00 Lunch Break

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Chair: Horst KÖPPEL

- 14:00 – 14:45** **Nimrod MOISEYEV** (Technion-Israel Institute of Technology)
Light induced conical intersections (REV3)
- 14:45 – 15:15** **Gerald AUBÖCK** (École Polytechnique Fédérale de Lausanne)
The Photochemistry of Iron Hexacyanide in Water (INV2)
- 15:15 – 15:40** **Regina DE VIVIE-RIEDLE** (LMU München)
Deceleration of dissociating molecular wave packets by solvent cage: the dynamic continuum ansatz (O03)
- 15:40 – 16:05** **Spiridoula MATSIKA** (Temple University of Philadelphia)
Dynamics on radical cations governed by conical intersections (O04)
- 16:05 – 16:45** Coffee Break

Chair: Wolfgang ERNST

- 17:00 – 18:00** **Karl Alexander MÜLLER** (University of Zürich)
Over half a century of research in oxides (PL)
- 19:00** **Reception at City Hall**

Tuesday, 19 August 2014

8:00 – 9:00 **REGISTRATION**

Chair: Miguel MORENO

- 9:00 – 9:45** **Jörg WRACHTRUP** (Stuttgart University)
Defects in Diamond: New Hardware for the Quantum World (REV4)
- 9:45 – 10:10** **Bin ZHANG** (Chinese Academy of Sciences, Beijing)
Organic-Inorganic Hybrid Dual-functional Molecular Crystal from Copper-Oxalate-Framework with Jahn-Teller Distortion (O05)
- 10:10 – 10:35** **Dennis P. CLOUGHERTY** (University of Vermont)
Dissipation and Decoherence of a Jahn-Teller Impurity in a Solid (O06)
- 10:35 – 11:15** Coffee Break

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Chair: Mihail ATANASOV

- 11:15 – 11:40** **Vladimir V.GUDKOV** (Ural Federal University, Ekaterinburg)
Evidence of magnetic field dependent relaxation in ZnSe:Cr crystal in ultrasonic experiment (O07)
- 11:40 – 12:05** **Kliment KUGEL** (Russian Academy of Sciences, Moscow)
Orbital and spin structures in transition metal compounds with face-sharing octahedral (O08)
- 12:05 – 12:30** **Simon NEVILLE** (University of Birmingham)
Multi-mode, Multi-State Quantum Dynamics Studies of Heteroaromatic Molecules (O09)
- 12:30 – 14:00** Lunch Break

Chair: Terry MILLER

- 14:00 – 14:45** **John F. STANTON** (The University of Texas at Austin)
Ground State of NO₂: From Lewis Structures to Spin-Orbit Coupling Effects (REV5)
- 14:45 – 15:15** **Mitchio OKUMURA** (California Institute of Technology, Pasadena)
Spectroscopy and Dissociation Dynamics of the Excited States of the Nitrate Cation NO₃⁺ (INV3)
- 15:15 – 15:40** **Matija ZLATAR** (University of Belgrade)
Computational Analysis of Intrinsic Distortions of Jahn-Teller and Pseudo Jahn-Teller Active Molecules (O10)
- 15:40 – 16:05** **Claude DAUL** (University of Fribourg)
Explicit Control Over Spin-states using combined Density Functional and Ligand Field Theory (O11)
- 16:05 – 16:30** Coffee Break

Chair: Spiridoula MATSIKA

- 16:30 – 16:55** **Daniel OPALKA** (University of Cambridge)
Construction of analytic multi-sheeted potential-energy surfaces from ab initio data (O12)
- 16:55 – 17:20** **David S. PERRY** (The University of Akron)
A System of e×E Conical Intersections Between Vibrationally Adiabatic Surfaces In Methanol (O13)
- 17:20 – 17:45** **Satrajit ADHIKARI** (Indian Association for the Cultivation of

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Science, Kolkata)

Conical Intersections in D_{3h} molecules: Diabatic PESs for Spectroscopic & Scattering Processes (O14)

18:00 Poster Session

Wednesday, 20 August 2014

8:00 – 9:00 REGISTRATION

Chair: Mitchio OKUMURA

9:00 – 9:45 Terry A. MILLER (The Ohio State University, Columbus)
Reconciliation of Spectroscopic Results and Electronic Structure Calculations for Jahn-Teller-Active Molecules (REV6)

9:45 – 10:30 Yuxiang MO (Tsinghua University, Beijing)
Jahn-Teller effect in CH₃X: spin-vibronic coupling, mode coupling and tunneling splitting (REV7)

10:30 – 11:00 Coffee Break

Chair: Wolfgang DOMCKE

11:00 – 11:30 Iain WILKINSON (National Research Council of Canada, Ottawa)
Sensitivities of Strong Laser Field Spectroscopies to Evolving Molecular Structure in Polyatomic Systems (INV4)

11:30 – 11:55 Camille LEVEQUE (UPMC Université Paris)
Ab initio quantum study of the photodynamics for the coupled 1^1A_2 and 1^1B_1 states of SO₂ (O15)

11:55 – 12:20 Sebastian MAI (University of Vienna)
Internal Conversion and Intersystem Crossing in SO₂ Studied by Surface-Hopping Molecular Dynamics (O16)

13:00 Departure for Conference Excursion:
Stift Vorau, Science Museum Pöllau

19:00 Conference Dinner

Thursday, 21 August 2014

8:00 – 9:00 REGISTRATION

Chair: Vladimir HIZHNYAKOV

9:00 – 9:45 Frank BRIDGES (University of California, Santa Cruz)

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Dynamic Jahn-Teller distortions in crystalline materials
(REV8)

9:45 – 10:30 **Pablo GARCÍA-FERNÁNDEZ** (Universidad de Cantabria, Santander)
Influence of Jahn-Teller and Pseudo Jahn-Teller over magnetism in 3d systems: A first-principles view (REV9)

10:30 – 11:15 Coffee Break

Chair: Claude DAUL

11:15 – 11:40 **Miguel MORENO** (Universidad de Cantabria, Santander)
Why the properties of K_2CuF_4 , $K_2ZnF_4:Cu^{2+}$ and $KZnF_3:Cu^{2+}$ model systems are so different? (O17)

11:40 – 12:05 **Annette BUSSMANN-HOLDER** (Max-Planck-Institut für Festkörperforschung, Stuttgart)
Probing spin fluctuations in the paramagnetic phase of $EuTiO_3$ by muon spin rotation techniques (O18)

12:05 – 12:30 **Grace MORGAN** (University College Dublin)
Broken Symmetry and Ordering Phenomena in Mn^{III} Spin Crossover Solids (O19)

12:30 – 14:00 Lunch Break

Chair: Frederic MERKT

14:00 – 14:45 **Martin JANSEN** (Max Planck Institute for Solid State Research, Stuttgart)
Fullerides: Radical Anions, Jahn-Teller Effect and Orbital Ordering (REV10)

14:45 – 15:10 **Erio TOSATTI** (International Centre for Theoretical Physics, Trieste)
Orbital excitation of a Mott-Jahn-Teller insulator revealed by infrared spectra (O20)

15:10 – 15:40 **Janette L. DUNN** (University of Nottingham)
Experimental signatures of Jahn-Teller effects in fullerene anions (INV5)

15:40 – 16:05 **Tohru SATO** (Kyoto University)
Regioselectivity in Chemical Reactions: Vibronic Coupling Density as a Reactivity Index (O21)

16:05 – 16:30 Coffee Break

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Chair: Lilia BOERI

- 16:30 – 17:00** **Liviu F. CHIBOTARU** (Katholieke Universiteit Leuven)
Dynamical Jahn-Teller instability in alkali-doped fullerenes
(INV6)
- 17:00 – 17:25** **Denis ARČON** (Jožef Stefan Institute, Ljubljana)
Jahn-Teller orbital glass in the Mott insulating parent state of the molecular superconductor Cs₃C₆₀ (O22)
- 17:25 – 17:50** **Katalin KAMARÁS** (Wigner Research Centre for Physics, Budapest)
Dynamic Jahn-Teller effect in IR spectra of expanded Cs₃C₆₀ fullerenes at low temperature (O23)
- 18:00** **Poster Session**

Friday, 22 August 2014

Chair: Janette DUNN

- 9:00 – 9:45** **Jamie WARNER** (University of Oxford)
Defects in graphene and the role of Jahn Teller reconstructions
(REV11)
- 9:45 – 10:15** **Ayan DATTA** (Indian Association for the Cultivation of Science, Kolkata)
Silicene: Its different from Graphene (INV7)
- 10:15 – 10:40** **Victor POLINGER** (University of Washington, Seattle)
Jahn-Teller-promoted superconductivity in cuprates and iron pnictides (O24)
- 10:40 – 11:15** **Coffee Break**

Chair: Markus AICHHORN

- 11:15 – 11:45** **Hiroyasu KOIZUMI** (University of Tsukuba)
Supercurrent generation in Cuprate: Spin-vortex model
(INV8)
- 11:45 – 12:10** **Lilia BOERI** (University of Technology, Graz)
Electron-phonon superconductivity in AP₃P compounds: From weak to strong coupling (O25)
- 12:10 – 12:35** **Takashi KATO** (Graduate School of Engineering, Nagasaki)
New interpretation of the role of vibronic interactions in superconductivity (O26)